AMENDMENTS TO THE SPECIFICATION:

Please amend the following passage of the specification appearing on p. 57, ln. 20-29:

Such formats include, but are not limited to, Protein Data Bank ("PDB") format (Research Collaboratory for Structural Bioinformatics; ~~http://www.rcsb.org/pdb/docs/format/pdbguide2.2/guide2.2_frame.html~~); Cambridge Crystallographic Data Centre format ~~(http://www.ccdc.cam.ac.uk/support/csd_doc/volume3/z323.html)~~; Structure-data ("SD") file format (MDL Information Systems, Inc.; Dalby et al., 1992, J. Chem. Inf. Comp. Sci. 32:244-255), and line-notation, e.g., as used in SMILES (Weininger, 1988, J. Chem. Inf. Comp. Sci. 28:31-36).   Methods of converting between various formats read by different computer software will be readily apparent to those of skill in the art, e.g., BABEL (v. 1.06, Walters & Stahl, ©1992, 1993, 1994~~; http://www.brunel.ac.uk/departments/chem/babel.htm~~.)